Determination of ground state properties in quantum spin systems by single qubit unitary operations and entanglement excitation energies

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(Dated: December 13, 2007)

We introduce a method for analyzing ground state properties of quantum many body systems, based on the characterization of separability and entanglement by single subsystem unitary operations. We apply the method to the study of the ground state structure of several interacting spin-1/2 models, described by Hamiltonians with different degrees of symmetry. We show that the approach based on single qubit unitary operations allows to introduce *"entanglement excitation energies"*, a set of observables that can characterize ground state properties, including the quantification of single-site entanglement and the determination of quantum critical points. The formalism allows to identify the existence and location of factorization points, and a purely quantum *"transition of entanglement"* that occurs at the approach of factorization. This kind of quantum transition is characterized by a diverging ratio of excitation energies associated to single-qubit unitary operations.

PACS numbers: 03.65.Ca, 03.67.Mn, 73.43.Nq, 75.10.Jm

arXiv:quant-ph/0611035v4 21 Dec 2007

I. INTRODUCTION

With the advent of quantum information theory, entanglement has been recognized as a fundamental physical resource, on equal footing with other fundamental resources such as energy and entropy. The relationships between these resources are being actively investigated, and it has been suggested that the entanglement properties in many-body systems may be characterized by suitably defined energy observables [1, 2]. Establishing *direct* connections between energy observables and entanglement is of interest because the former could lead to a deeper conceptual understanding of the latter and be exploited for its experimental production and manipulation in complex quantum systems. On the other hand, the study of the role played by entanglement in quantum phase transitions [3, 4, 5] and its relations with ground state (GS) properties has sparked a rapidly growing field of research [6]. As entanglement plays a fundamental role in quantum information [7], the question then arises whether it is possible to determine structural aspects of complex quantum systems using concepts and techniques of quantum information theory. Relevant open challenges include the understanding of the relation between GS entanglement, physical observables, and criticality, as well as the determination of factorization points at which quantum ground states become separable [8, 9].

Recently, a formalism of *single subsystem unitary operations* has been introduced [10, 11]: These operations are defined as unitary and traceless local transformations with non degenerate spectrum (as well as Hermitian, in the case of qubits) that act on a single subsystem, leaving unaffected the remaining ones. The corresponding approach provides a tool for studying pure state entanglement for systems of qubits (spin 1/2) or qutrits (spin 1) [10], and for Gaussian states of continuous variable systems [11]. For such systems, a necessary and sufficient condition for pure state separability is the existence of a unique transformation (termed *invariant*) that leaves the state unchanged. On the other hand, if a pure state is entangled, the minimum Euclidean distance in Hilbert space from the state and its image under the action of single subsystem unitary operations singles out a unique, *extremal* operation that is directly related to the entanglement properties of the state. Namely, the squared minimum distance coincides exactly with the linear entropy, and is thus monotone in the entropy of entanglement of the state. As a consequence of these results, separability points are determined and singled out by imposing equality of the extremal and invariant operations.

The approach based on single subsystem unitary operations allows to gain informations on the global nature of pure states of a composite system by looking at how states transform under local operations that, by definition, do not change the content of entanglement (local unitaries). Moreover, the method finds a natural operational interpretation, as looking at the response to a given action is a basic tool in the investigation of physical properties.

The structure of the paper is as follows: In Sec. II we introduce Single Qubit Unitary Operations (SQUOs), and show that each SQUO singles out a direction in the

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three-dimensional single-spin space; we then define the *extremal* SQUO, as the one associated to the distance of the ground state (GS) from the nearest state in the set of states obtained from the GS under the action of SQUOs. In Sec. III, we define the excitation energy relative to each SQUO, and demonstrate that, under rather general conditions, the excitation energy associated with the extremal SQUO vanishes if and only if the GS is factorized: We therefore name it *entanglement excitation energy* (EXE). Sec. IV is devoted to the analysis of several $S = 1/2$ one-dimensional spin models, with attention focused on the dependence of the EXE on the Hamiltonian parameters. In Sec. V we present and discuss our results: we find that the EXE follows monotonically the behavior of the GS single-site entanglement (i.e. the von Neumann block entropy between a single spin and the rest of the system) and exhibits signatures of the relevant GS properties, including the existence and location of factorization and quantum critical points. Finally, we introduce the *orthogonal* SQUOs as those defined by two directions orthogonal to each other, and to the direction selected by the extremal SQUO: We find that the corresponding excitation energies coincide when the EXE vanishes, in such a way that the ratio between their difference and the EXE itself diverges at the approach of a factorization point in a large class of models: such a divergence may therefore be exploited in order to detect the *entanglement transition* associated with the occurrence of a fully separable ground state [12, 13] in strongly correlated quantum systems. In Sec. VI we draw our conclusions and discuss some possible future lines of research.

II. SINGLE QUBIT UNITARY OPERATIONS

Consider a N-qubit system. A SQUO is defined [10] as the following unitary transformation

$$U_k \equiv \bigotimes_{i\neq k} \mathbf{1}_i \otimes \mathcal{O}_k \ , \tag{1}$$

where the operators $\mathbf{1}_i$ are the identities on the $N-1$ spins different from spin k, and the operator $\mathcal{O}_k$ is a Hermitian, unitary, and traceless 2×2 transformation, acting on spin k. In the standard basis $\{|\uparrow\rangle, |\downarrow\rangle\}$, $\mathcal{O}_k$ is parametrized as

$$\mathcal{O}_k(\theta,\varphi) = \begin{pmatrix} \cos\theta & \sin\theta e^{-i\varphi} \\ \sin\theta e^{i\varphi} & -\cos\theta \end{pmatrix} , \tag{2}$$

where θ and φ vary in the ranges $[-\pi/2, \pi/2)$ and $[0, 2\pi)$, respectively. The above expression may be written as $\mathcal{O}_k = u \cdot \boldsymbol{\sigma}_k$, where $\boldsymbol{\sigma}_k = (\sigma_k^x, \sigma_k^y, \sigma_k^z)$ are the Pauli matrices, and the unitary vector $u \equiv (u_x, u_y, u_z) = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$ defines a direction in the three-dimensional single-spin space: each direction in such a space defines a SQUO and, viceversa, to each SQUO there corresponds one such direction. The action of a SQUO transforms any pure state $|\Psi\rangle$ defined in the 2^N dimensional Hilbert space in the state $U_k|\Psi\rangle$. If $U_k|\Psi\rangle = |\Psi\rangle$ then U_k is the *invariant* SQUO. In general, however, the transformed state differs from $|\Psi\rangle$: This difference can be quantified by introducing the standard Hilbert-Schmidt distance:

$$\begin{aligned} d(U_k; |\Psi\rangle) &\equiv \sqrt{1 - |\langle\Psi|U_k|\Psi\rangle|^2} = \\ &= \sqrt{1 - |\langle\Psi|u\cdot\boldsymbol{\sigma}_{\boldsymbol{k}}|\Psi\rangle|^2} \equiv d(u; |\Psi\rangle) \ . \end{aligned} \tag{3}$$

Minimizing the distance over the entire set of SQUOs, i.e. evaluating $\min_{\{\theta,\varphi\}} d(u; |\Psi\rangle)$, yields that the distance of a pure state from the nearest transformed state is obtained for [10]:

$$\begin{aligned} \widetilde{\varphi} &= \arctan\left(\frac{M_k^y}{M_k^x}\right) , \\ \widetilde{\theta} &= \arctan\left(\frac{M_k^x\cos\widetilde{\varphi} + M_k^y\sin\widetilde{\varphi}}{M_k^z}\right) , \end{aligned} \tag{4}$$

where M_k^α denotes the spin expectation values $\langle\sigma_k^\alpha\rangle/2$ ($\alpha = x, y, z$) on the state $|\Psi\rangle$. The values (4) fix the direction $\widetilde{u}$ which determines the *extremal* SQUO, U_k^{extr}. The distance $d(\widetilde{u}; |\Psi\rangle)$ of a state from the nearest transformed state, corresponding to the extremal SQUO U_k^{extr}, can be evaluated explicitly, and its square reads

$$d^2(\widetilde{u}; |\Psi\rangle) = 1 - \left[(M_k^x)^2 + (M_k^y)^2 + (M_k^z)^2\right] \ . \tag{5}$$

This is exactly the linear entropy S_L of state $|\Psi\rangle$: $S_L = 2(1 - \mathrm{Tr}[\rho_k^2])$, where ρ_k is the single-site reduced density matrix after tracing out the $N-1$ remaining spins. It is a well known fact that in the case of qubits the linear entropy coincides with the tangle τ: $S_L = \tau \equiv 4\mathrm{Det}\rho_k$ [14, 15]. The pure state entanglement, measured by the von Neumann entropy $\mathcal{E}$ [16], is a single-valued, monotonic function of either of these two coinciding quantities (either the linear entropy or the tangle): $\mathcal{E}(|\Psi\rangle) = -x\ln_2 x - (1-x)\ln_2(1-x)$ where $x = (1+\sqrt{1-\tau})/2$. Therefore, due to Eq. (5), extremal SQUOs and the associated Euclidean distances determine pure state entanglement, whose entropic quantification is recast in direct geometric terms.

III. ENTANGLEMENT EXCITATION ENERGIES

The full consequences of the above results can be exploited for the characterization of GS properties. In the following, we show that U_k^{extr} can be used to construct an energy observable which witnesses GS separability and quantifies GS entanglement.

Let $|G\rangle$ be the GS of a system of interacting spins with Hamiltonian $\mathcal{H}$, and define the excitation energies,

$$\Delta E(U_k) \equiv \langle G|U_k^\dagger \mathcal{H} U_k|G\rangle - \langle G|\mathcal{H}|G\rangle \ ; \tag{6}$$

the dependence of $\Delta E(U_k)$ on the parameters θ and φ, i.e. on the direction u selected by the SQUO U_k, is made evident by using Eqs. (1) and (2). One obtains that

$$\begin{aligned} \Delta E(U_k) \;=\; & u_x^2 \Delta E(\sigma_k^x) + u_y^2 \Delta E(\sigma_k^y) + u_z^2 \Delta E(\sigma_k^z) + \\ & + u_x u_y \epsilon_{xy} + u_x u_z \epsilon_{xz} + u_y u_z \epsilon_{yz} \;, \end{aligned} \tag{7}$$

where $\epsilon_{\alpha,\beta} = \epsilon_{\beta,\alpha} \equiv \langle G|\sigma_k^\alpha \mathcal{H} \sigma_k^\beta + \sigma_k^\beta \mathcal{H} \sigma_k^\alpha |G\rangle$.

Amongst these excitation energies, which are non-negative by definition, the one corresponding to the extremal SQUO, $\Delta E(U_k^{extr})$, has a prominent role in the analysis of entanglement properties of the GS, due to the intimate relation between its vanishing and the occurrence of full separability. We will therefore name it *entanglement excitation energy* (EXE).

In fact, if in the GS the spin k is not entangled with the rest of the system, then $U_k^{extr}|G\rangle = |G\rangle$, and the EXE consequently vanishes. On the other hand, if the spin k is entangled with the rest of the system, one necessarily has $U_k^{extr}|G\rangle \neq |G\rangle$ and the EXE may vanish only if $U_k^{extr}|G\rangle$ is again a state of minimum energy, i.e. if $\langle G|[\mathcal{H}, U_k^{extr}]|G\rangle = 0$. Therefore, barring pathological or trivial cases in which the Hamiltonian does commute with each SQUO, the vanishing of the EXE occurs only in the presence of a factorized GS, proving the statement.

It is worth noticing that the vanishing of the EXE is a necessary, but not sufficient, condition for the separability of excited states. In fact, considering an entangled excited state $|\psi\rangle$, the action of the corresponding extremal SQUO transforms it in a different state that is not, in general, an eigenstate of the Hamiltonian and can have a non vanishing projection on any possible eigenstate of the system. The possibility to populate eigenstates with energy lower than that associated to $|\psi\rangle$ makes then it possible to obtain a vanishing EXE even in the presence of an extremal SQUO.

IV. INTERACTING SPIN SYSTEMS

Equipped with these results, we move on to apply them to the determination of the GS properties of interacting spin systems. We consider antiferromagnetic anisotropic Heisenberg-like XYZ model Hamiltonians:

$$\mathcal{H} = \sum_i S_i^x S_{i+1}^x + \Delta_y S_i^y S_{i+1}^y + \Delta_z S_i^z S_{i+1}^z - h S_i^z \;, \tag{8}$$

where $S_i^\alpha = \sigma_i^\alpha/2$, the index i runs on the sites of a one-dimensional lattice, and periodic boundary conditions are assumed. In Eq. (8) h is the reduced (dimensionless) magnetic field, and Δ_y, Δ_z are the anisotropy parameters, $0 \leq \Delta_{y,z} \leq 1$. This choice is motivated by its great generality: according to the different values of the anisotropies, Eq. (8) comprises many different models belonging to different classes of universality, including the Ising and the Heisenberg ones. For the models described by Eq. (8) genuine quantum phase transitions, with or without order parameter, occur at zero temperature at critical values $h_{\rm c}$ that depend on the anisotropies. If $\Delta_y = 1$, the symmetry forces a transition without order parameter, and the system remains in a critical regime for all $h \leq h_{\rm c}$. In this case if $\Delta_z \neq 1$ the system is in the XXZ symmetry class and goes over to the Heisenberg symmetry class when $\Delta_z = 1$. For $0 \leq \Delta_y < 1$, the system undergoes a second order phase transition, acquiring a non-vanishing staggered magnetization along the x direction for $h < h_{\rm c}$. Antiferromagnetic order divides the lattice in two sublattices, each characterized by opposite value of the magnetization. Again, changing the value of Δ_z lets the system move from the Ising symmetry class ($\Delta_z = 0$) to the XYZ symmetry class ($\Delta_z \neq 0$). Concerning the magnetization along the directions y and z, one has that, regardless of the anisotropy, the magnetization M_y is always vanishing, while M_z vanishes at and only at $h = 0$. Importantly, in the models described by Eq. (8) the external field not only drives the system through a quantum phase transition, but induces as well the factorization of the GS, for $h = h_{\rm f} \equiv \sqrt{(1+\Delta_z)(\Delta_y+\Delta_z)}$ [8]. This phenomenon has been recently investigated in relation to the analysis of entanglement properties in spin systems [9]. For the ground states of the models described by Eq. (8), the vanishing of the EXE is a necessary and sufficient condition for GS separability.

Using Eqs. (4), and considering that it is always $M_k^y = 0$, and hence $\widetilde{\varphi} = 0$, on gets, by Eq. (7), the exact expression of the EXE that reads

$$\begin{aligned} \Delta E(\widetilde{u}) \;\equiv\; & \Delta E(U^{extr}) = \\ =\; & -16 \left[\frac{g_{xx} M_z^2 - M_x M_z g_{zx}}{1-\tau} + \frac{\Delta_y g_{yy}}{4} \right. \\ & \left. + \frac{\Delta_z \left(g_{zz} M_x^2 + M_x M_z g_{zx} \right)}{1-\tau} \right] \;, \end{aligned} \tag{9}$$

where $\tau = S_L$ is the GS tangle (linear entropy), $g_{\alpha\beta} = \langle G|S_i^\alpha S_{i+1}^\beta|G\rangle$ are the nearest-neighbor correlation functions, $M_\alpha = \langle G|S_i^\alpha|G\rangle$ are the expectation values of the spin operators, and any dependence on the site index is neglected due to translational invariance.

V. RESULTS

We first analyze the EXE, $\Delta E(\widetilde{u})$, and compare it with the von Neumann entropy $\mathcal{E}$. The latter measures the bipartite single-site entanglement between one selected spin and the rest of the chain [16], and it provides an upper bound to all bipartite block entanglements. Therefore, its vanishing guarantees the full separability of the GS. Exploiting the conditions for the vanishing of S_L and $\Delta E(\widetilde{u})$ allows to determine unambiguously the value and location of the factorization point.

In Figs. 1 and 2 we plot $\Delta E(\widetilde{u})$ and $\mathcal{E}$ as functions of h. Fig. 1 shows exact analytical results [17, 18] for the XY model, and Quantum Monte Carlo (QMC) data for the

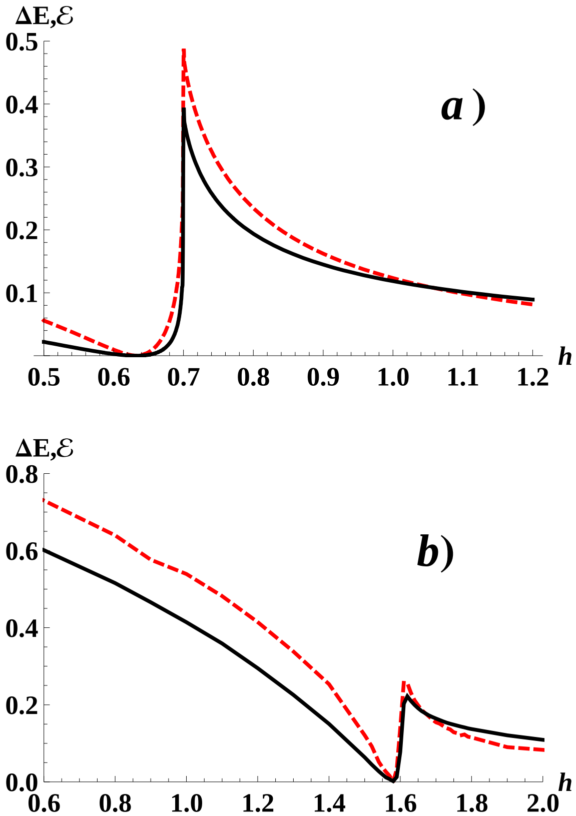

FIG. 1: (color online) Entanglement excitation energy $\Delta E(\widetilde{u})$ (Black solid line) and single-site entanglement $\mathcal{E}$ (Red dashed line) as functions of the reduced field h, for *a)*: $\Delta_y = 0.4$, $\Delta_z = 0$ (XY), and *b)*: $\Delta_y = 0.25$, $\Delta_z = 1$ (XYZ). All quantities are dimensionless.

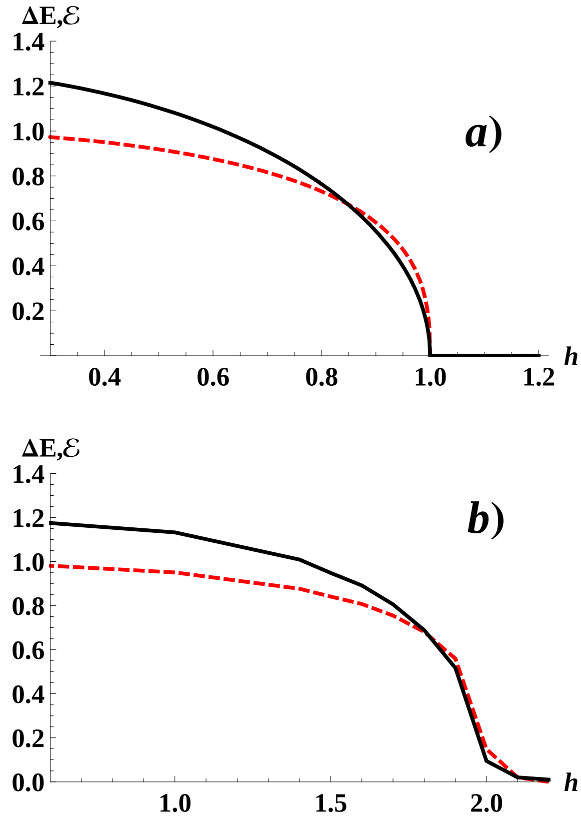

FIG. 2: (color online) Entanglement excitation energy $\Delta E(\widetilde{u})$ (Black solid line) and single-site entanglement $\mathcal{E}$ (Red dashed line) as functions of the reduced field h, for *a)*: $\Delta_y = 1$, $\Delta_z = 0$ (XXZ), and *b)*: $\Delta_y = 1$, $\Delta_z = 1$ (Heisenberg). All quantities are dimensionless.

XYZ model. Fig. 2 shows exact analytical results [17] for the XX model, and QMC data for the Heisenberg model. Numerical data have been obtained via stochastic-series-expansions quantum Monte Carlo simulations [9, 19], based on a modified directed-loop algorithm. The EXE and the entropy of entanglement evidently exhibit the same behavior, vanishing simultaneously at the factorization points. At critical points, the derivatives of both $\Delta E(\widetilde{u})$ and $\mathcal{E}$, with respect to h, diverge, signaling the onset of a quantum phase transition. This divergence occurs both for $\Delta_z = 1$ and $\Delta_z < 1$, at variance with the concurrence, i.e. a measures of the entanglement between two spins of the lattice [20], that exhibit different behaviors at the critical points for models with different symmetries [6]. In this sense, we suggest that the EXE, contrary to other observable estimators of entanglement, can be considered a *universal* indicator for the onset of quantum phase transitions in spin systems.

The relevance of SQUOs and EXEs in determining entanglement and factorization properties, and in general qualitative changes in the GS can be understood in physical terms and related to "entanglement transitions"[12, 13]. If a system is in a pure classical state the orientation of any spin is well defined. Selecting a spin and performing a rotation about its orientation leaves the state of the system and its energy unchanged. Viceversa, if the system is in an entangled quantum state the single-spin orientation is not defined and any "rotation" , i.e. any SQUO, will change the state of the system and will yield a change in energy. Therefore, the increase in energy is connected to "how much the GS is entangled" . Constructing the excitation energy associated to the extremal SQUO, i.e. the EXE, formalizes the argument.

Based on the above comparison with the classical case, let us introduce two directions, $u'_\perp$ and $u''_\perp$, orthogonal to each other and to the direction $\widetilde{u}$ associated to the extremal SQUO U^{extr}. Being $\widetilde{u} = (\sin\widetilde{\theta}, 0, \cos\widetilde{\theta})$, we choose $u'_\perp = (\cos\widetilde{\theta}, 0, -\sin\widetilde{\theta})$ and $u''_\perp = (0,1,0)$. These directions define the *orthogonal* SQUOs, via Eq. (2), and the corresponding excitation energies $\Delta E'_\perp$ and $\Delta E''_\perp$, via Eq. (7). In Fig. 3 we compare the field dependence of the EXE with that of the above defined excitation energies, for the XY and XYZ models: We find that $\Delta E'_\perp$ and $\Delta E''_\perp$ coincide at $h_{\rm f}$, i.e. when the GS is factorized, in full analogy with the classical case. In fact if the system is in a pure classical state any rotation of $\pi/2$ around a direction orthogonal to the spin orientation causes an in-

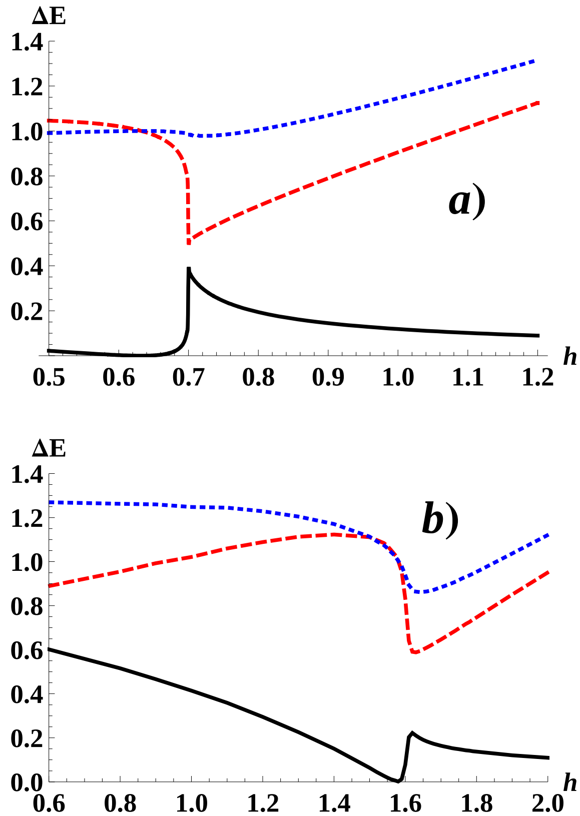

FIG. 3: (color online) Entanglement excitation energy $\Delta E(\widetilde{u})$ (Black solid line), excitation energy $\Delta E'_{\perp}$ (Red dashed line), and excitation energy $\Delta E''_{\perp}$ (Blue dotted line) as functions of h, for *a)*: $\Delta_y = 0.4$, $\Delta_z = 0$ (XY), and *b)*: $\Delta_y = 0.25$, $\Delta_z = 1$ (XYZ). All quantities are dimensionless.

crease in energy by one (in units of the reduced field). For $h \neq h_f$, $\Delta E'_{\perp}$ and $\Delta E''_{\perp}$ behave differently, a fact which has no classical analogue, so that the deviation from classicality can be quantified by the difference $\Delta E'_{\perp} - \Delta E''_{\perp}$.

We can then compare such difference to the amount of entanglement, as measured by the EXE, by defining the *entanglement energy ratio* (EER)

$$R_E = \frac{\Delta E'_{\perp} - \Delta E''_{\perp}}{\Delta E(\widetilde{u})} \, . \tag{10}$$

In Fig. 4 we show the behavior of the EER R_E, as a function of h, for two models belonging, respectively, to the XY and to the XYZ universality class. In both cases, R_E diverges at the factorization point h_f, and its first derivative diverges at the critical point h_c. The abrupt change in the GS properties at the factorization point, as measured by the divergence of the EER, signals a qualitative change of purely quantum nature, a "transition of entanglement" that occurs when h_f is approached. We remark that all the conventional on-site expectations and n-point correlation functions remain finite and analytic at a factorization point, confirming that the divergence of the EER cannot be associated to any kind of conventional quantum phase transition. On the other hand, the

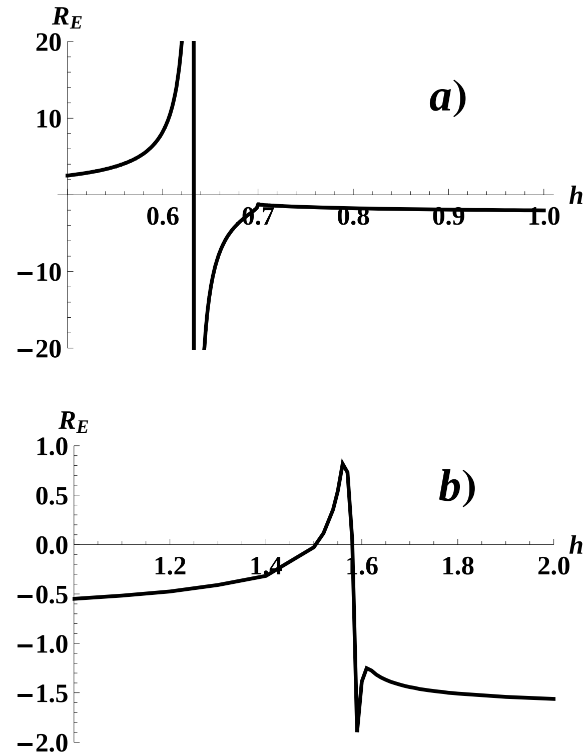

FIG. 4: (color online) Entanglement energy ratio R_E as a function of h, for *a)*: $\Delta_y = 0.4$, $\Delta_z = 0$ (XY), and *b)*: $\Delta_y = 0.25$, $\Delta_z = 1$ (XYZ). All quantities are dimensionless.

EER remains fixed at the constant value $R_E = -1$ if we consider models of interacting spins with $\Delta_y = 0$: The fact that in this case the EER fails to identify the transition from entanglement to factorizability is intriguing and deserves further studies.

VI. CONCLUSIONS AND OUTLOOK

In summary, we have defined entanglement excitation energies (EXEs) associated to the extremal single qubit unitary operations (SQUOs). We have showed that EXEs are useful tools for the study of various ground state properties for interacting spin systems, including the determination of factorizability, the quantification of single-site entanglement, and the identification of quantum critical points. We have discussed how SQUOs and EXEs determine unambiguously the presence or the absence of a separable GS, and we have introduced an entanglement energy ratio (EER) of excitation energies that diverges (for $\Delta_y \neq 0$) at the approach of a factorization point, thus defining an entanglement-separability transition of purely quantum origin.

Considering possible future developments along this line of research, we would like to observe that when moving away from the factorization point, the physics of quantum ground states can in principle be recovered by expanding the single-site entanglement in powers of

the EXE, as the latter naturally defines a small expansion parameter of the theory around a factorization point. The analytic generalization of the formalism to general spin models is a subject of current investigation. The results of such an analysis could allow to determine exact solutions of non exactly solvable models at factorization points, as well as the approximate description of GS properties out of the factorization point by controlled expansions in powers of the EXEs. The necessary and sufficient conditions for factorizability obtained within the formalism of SQUOs might be extended to the case of models involving interacting systems of arbitrary local dimension. In particular, it would be very interesting to consider interacting systems of very high spins and study them in a continuous-variable representation, for which single-subsystem unitary operations can be readily expressed in terms of single-mode unitary transformations. This line of investigation could then be extended as well to include models of interacting harmonic and anharmonic chains and lattices.

Conceptually, the present work discloses an intimate connection between two different universal physical resources, energy and entanglement, and might have practical consequences for the experimental production and manipulation of entanglement, and information transfer in real systems of interacting qubits. The single-qubit excitation energy provides a well-defined form of macroscopic observable for the detection and determination of single-site entanglement in many-body systems, along lines close in spirit to pair-entanglement detection in systems of interacting magnetic dipoles by measurements of heat capacities and magnetic susceptibilities [21]. As a working example, the method has been applied and illustrated in quantum spin-1/2 models, that are of particular relevance both for quantum information and condensed matter physics. However, in principle it can be applied as well to more general instances [10, 11], such as systems of interacting qutrits, Hubbard models, and harmonic lattices of continuous variables. The choice of nearest-neighbor couplings in the case of interacting qubits deserves a comment. In fact, the method is in no way limited by the choice of the interaction. Generalizations to spin models with interactions of arbitrary range and lattices of different topologies are possible and, as suggested above, can be of particular relevance in establishing the existence of factorization points and in constructing consistent descriptions of GS quantum physics by systematic expansions in powers of the EXE around the factorized solutions.

VII. AKNOWLEDGEMENTS

We are grateful to Tommaso Roscilde for providing us with relevant Quantum Monte Carlo data. SMG and FI wish to thank Rosario Fazio for helpful discussions. This work was supported by MIUR under the 2005-2007 PRIN-COFIN National Project Program, CNR-INFM Coherentia, ISI Foundation, and INFN.

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